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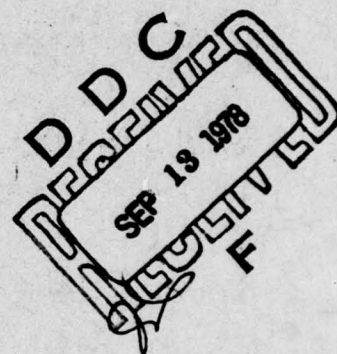
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QUANTUM THEORY OF MATTER - COHESIVE AND SPECTRAL PROPERTIES

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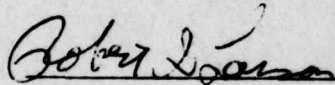
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FOREWORD

Contract number AFOSR-75-2753, AFAL-TR-77-263, Quantum Theory of Matter - Cohesive and Spectral Properties, performed by Per-Olov Löwdin, Professor of Physics, University of Uppsala at S-751 20 Uppsala, Sweden. This contract monitored by Dr. T. C. Collins, Aerospace Research Laboratories, Wright-Patterson Air Force Base, Ohio. Research performed during the period 1 July 1974 - 30 June 1975, by Per-Olov Lowdin with the assistance of Prof. J. L. Calais, Prof. O. Goscinski, and Prof. Dennis Caldwell.

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TABLE OF CONTENTS

	Page
I. INTRODUCTION	1
II. THEORETICAL CONSIDERATIONS FOR COHESIVE PROPERTIES OF SOLIDS	7
III. TRANSITION OPERATORS FOR DESCRIBING IONIZATION AND EXCITATION.....	9
IV. COMPUTATIONAL METHODS FOR ABSORPTION AND MAGNETIC CIRCULAR DICHROISM INTENSITIES	11

I. INTRODUCTION

Part of the interest during this period has been concentrated on the electronic structure of solids: the behaviour of the alkali halides and similar crystals under very high pressure (p-116), the removal of approximate linear dependencies in the MO-LCAO-approach (p-117), and the treatment of the correlation effects in the free-electron gas using the alternant-molecular-orbital approach (p-118). None of these studies has been fully concluded, and continued research on these problems is still going on.

The main interest during this period has been devoted to the foundations of quantum mechanics, and particularly to the following two problems:

- a) the combination of special relativity and quantum mechanics to a unified theory including also many-electron systems
- b) the combination of electronic physics and chemistry - classical mechanics, thermodynamics, quantum statistics, and quantum mechanics - into a single theory.

In connection with the first problem, it has been possible to show that one can derive the entire structure of the special theory of relativity without mentioning the phenomenon of light. The Lorentz-transformations obtained in this way contain a fundamental constant " a " which has the character of a "limit velocity" in the theory. Using these transformations, one may now develop a wave mechanics without the introduction of Planck's constant " h ". If there is a wave-modulating field - corresponding to "classical forces" - there are standing waves only under certain conditions corresponding to Schrödinger's original idea of "quantization as an eigenvalue problem". In this way, one finds that the quantization of the hydrogen atom associated with the Coulomb field is regulated by a coupling constant α which is identical to the fine-structure constant

(MS1). So far, no method has been found to determine its value.

The relativistic formulas obtained correspond to the Dirac formulas for a particle without spin, and they differ hence slightly from the Sommerfeld formulas. Using ideas from the Dirac theory, one may also introduce "spin properties" of the essentially classical waves under consideration.

It seems rather clear that, whatever approach one is using for combining special relativity and quantum mechanics, one may finally need infinite linear spaces having an indefinite metric.

Part of the purpose of the relativistic studies is to find the correct "relativistic corrections" also for the heavier atoms in the periodic system, and it is believed that this may be of essential importance both in quantum chemistry and solid-state physics. So far, little progress has been made on this fundamental problem, and more intense studies are planned for the future.

In the theory of chemical kinetics, the incoming particles are usually classically described whereas the collision process is treated by means of quantum mechanics. Since the temperature is also of importance, it is desirable to include both classical thermodynamics as well as quantum statistics. All these theories may be unified in a "trace algebra" (MS2). The system is described by a density operator Γ in the Liouville space, which undergoes a similarity transformation with time "t". All the fundamental formulas in electronic physics and chemistry - as well as quantum mechanics - are easily derived, and one may study stationary states, equilibrium states, and the approach to equilibrium. By means of the similarity transformation, reversible and irreversible processes are clearly defined, and one may derive the equation of state as well as the second law of thermodynamics. The idea is to apply this unified approach to the theory of chemical kinetics and particularly to quantum biology.

The uncertainty relations in the trace algebra (MS3) contain Heisenberg's uncertainty relations as a special quantum-

mechanical case, but they represent also an interesting generalization of importance for the particle concept.

The trace algebra is formulated in an operator space, the carrier space of which may be either positive definite or indefinite. The latter possibility may be of essential importance in treating relativistic phenomena.

In connection with chemical kinetics, there is also a great interest in collision phenomena. Among mathematicians, it is a well-known fact that the quantum-mechanical "transformation theory" as formulated by e.g. Dirac is not mathematically rigorous, and that the Fourier-transformations cannot as a rule be applied to Hilbert spaces and that the correct transformation is the Fourier-Plancherel one. The corresponding transformations associated with a general observable having a discrete and continuous spectrum have been studied in some detail (MS4), and the results are being applied to the study of discrete states embedded in the continuum as well as to free particles.

Since in quantum chemistry and solid-state physics, one has often to use truncated basis sets, a special "error quotient" measuring the degree of completeness has been introduced and practically studied (MS5).

In conclusion, it should be mentioned that some interest has been devoted to the standard Hartree-Fock scheme using completely general spin orbitals (GSO), and that some new results have been obtained (MS6). This is a preliminary study which will lead over to a more detailed study of the projected Hartree-Fock (PHF) scheme using general spin-orbitals, which may be of practical importance for the study of the electronic structure of atoms, molecules, and crystals. It is believed that this general PHF-scheme will give the major part of the conventional correlation error and hence render a simple scheme for treating most problems in the theory of the electronic structure of stationary states of atoms, molecules, and crystals.

Even the philosophical aspects of the development of the theory have been at least partly covered (P-120, TN-462),

and the mathematical tools have been given a new treatment with particular emphasis on methods general enough to permit also the inclusion of spaces having an indefinite metric (TN-472).

Practically all of the ideas presented here represent only starting points for research which has to be continued over many years to come. The results obtained so far are enough promising to encourage us to go on along the lines briefly outlined above.

SOME RECENTLY PUBLISHED PAPERS: P.O. LÖWDIN

- P-116. (together with J.-L. Calais and M. Hayns)
A Theoretical Study of the Behaviour of Solids under
High Pressure and the Borelius Law, with Applications
to the Alkali Halides.
(J. of Nonmetals, 1, 63-78, 1972).
- P-117. (together with T. Ahlenius, J-L Calais). Some Com-
ments on the Construction of an Orthonormal Set of
LCAO Basis Functions for Crystals.
(J. Phys. C: Solid State Phys. 6, 1896, 1973).
- P-118. (together with B. Laskowski, J-L Calais, P.V. Leuven).
Electron Gas Test for the Alternant Molecular Orbital
Method.
(J. Phys. C: Solid State Phys. 6, 2777, 1973).
- P-119. "Josef-Maria Jauch", In Memoriam;
(Europhysics News 5, 7, 1974).
- P-120. "Människan och hennes psyke i den moderna kvantteorins
världsbild".
(Forskning och Framsteg, vol. 6, nr. 10, 1974).

RECENTLY ISSUED PREPRINTS: P.O. LÖWDIN

- TN 462: "Some Aspects on Objectivity and Reality in Modern
Science", 59 pages, September 1975.
- TN 472: "Set Theory and Linear Algebra - some Mathematical
Tools to be Used in Quantum Theory", ... pages, Sep-
tember 1975.
- TN 470: "Some Aspects on the American-Swedish Exchange in
Quantum Sciences - particularly the Uppsala-Florida
Exchange Project", ... pages, December 1975.
(to be published in the Swedish Foreign Department
tributary volume to the U.S. Bicentennial celebration).
- TN 471: "Internationella aktiviteter å Kvantkemiska Institu-
tionen och Forskargruppen vid Uppsala Universitet" -
- för publicering i "Universen", November 1975.

PAPERS PREPARED IN MANUSCRIPT: P.O. LÖWDIN

- MS1. "Wave Mechanics and the Special Theory of Relativity".

- MS2. "Unification of Electronic Physics and Chemistry as a Trace Algebra".
- MS3. "A Generalization of the Uncertainty Relations based on the Trace Algebra".
- MS4. "The Transformation Principle in the Theory of the Hilbert Spaces; Rigorous Treatment of the Eigenfunctions in the Continuum".
- MS5. "Error Quotient; a Simple Measure of the Completeness of Truncated Basic Sets".
- MS6. "Hartree-Fock Scheme Using General Spin-Orbitals".

II. THEORETICAL CONSIDERATIONS FOR COHESIVE PROPERTIES OF SOLIDS

Jean-Louis Calais

The theory of cohesive properties of solids is at the crossing point of the two main branches of solid state physics: lattice dynamics and electronic structure. So far each one of them have developed relatively independently, and a detailed quantitative tie between them is still lacking. It seems plausible that at least one reason for this is the lack of a consistent and quantitatively reliable theory of cohesive properties.

Some of the first really detailed quantum mechanical calculations of cohesive and elastic properties of ionic crystals were carried out by Löwdin in Uppsala in the 1940's. Such calculations were taken up again and extended in the Uppsala Quantum Chemistry Group in the middle of the sixties. Although the results are on the whole relatively satisfactory, it is definitely desirable to go beyond the approximations invoked in these investigations.

A number of new tools have recently become available, which seems to make a new attack on these problems worthwhile. Apart from the many improvements in computer programs for molecular integrals, there are two new theoretical procedures which seem very promising. First Ra has taken up the problem of calculating the inverse of the overlap matrix - a central point in the LCAO method used in all these calculations. His analysis has led to a new power series for this matrix, which converges much more rapidly than the geometric series used so far. Secondly, Kohn has taken up and developed a variational principle proposed by Koster in 1953 for the direct calculation of Wannier functions. This procedure seems to open up interesting possibilities for getting better approximations to the Wannier functions than the orthogonalized atomic orbitals of the free ions, which have been used so far.

A more detailed survey is given in paper 7 in the following list of publications.

Publications by J-L Calais during the period 1973-75.

(Printed papers; mimeographed reports; manuscripts).

1. J.-L. Calais och G. Sperber, "A Study of the AMO Method as Applied to the Lithium Metal. I. Review, results, discussion". Int. J. Quantum Chem. 7, 501 (1973).
2. G. Sperber och J.-L. Calais, "A Study of the AMO Method as Applied to the Lithium Metal. II. The First-Order Density Matrix and the Shape of the Fermi-Surface". Int. J. Quantum Chem. 7, 521 (1973).
3. T. Ahlenius, J.-L. Calais och P.-O. Löwdin, "Some Comments on the Construction of an Orthonormal Set of LCAO Basis Functions for Crystals". J. Phys. C 6, 1896 (1973).
4. B. Laskowski, J.-L. Calais, P.-O. Löwdin och P. Van Leuven, "Electron Gas Test for the Alternant Molecular Method", J. Phys. C 6, 2777 (1973).
5. M.-R. Hayns och J.-L. Calais, "Cohesive Energy of Silver Fluoride", J. Phys. C 6, 2625 (1973).
6. J.-L. Calais, "Electronic Correlation in Polymers and Molecular Crystals", Electronic Structure of Polymers and Molecular Crystals (Ed. J-M André and J. Ladik, Plenum Press, New York and London 1975), p. 389.
7. J.-L. Calais, "Cohesive Properties of Ionic Crystals", Int. J. Quantum Chem. 9S, 000 (1975).
8. A.H. Tang Kai och J.-L. Calais, "Calculation of the Electronic Structure of Ethylene by the SCF-X α Scattered Wave Method", Theor. Chim. Acta (1975).
9. M. Larsson, S. Byström och J.-L. Calais, "Program to Compute SAPW-Bands from an APW-Potential", Upsala University, Institute of Physics, Report 854, March 1974.
10. S. Byström, M. Larsson och J.-L. Calais, "Band Structure of CoSn by the SAPW Method", Upsala University, Institute of Physics, Report 862, March 1974.
11. J.-L. Calais, "Band Structure of Solids", October 1974.
12. B. Laskowski, P. Van Leuven och J.-L. Calais, "Alternant Molecular Orbital Excitations by the Generator Coordinate Method in the Electron Gas", Physica 80A, 561 (1975).
13. J.-L. Calais, "Many Electron Theory", July 1975.
14. J.-L. Calais, "Some Comments on the Quantum-Mechanical Treatment of Static Defects in Ionic Crystals", October 1975.

III. TRANSITION OPERATORS FOR DESCRIBING IONIZATION & EXCITATION

Oswaldo Goscinski

The work summarized in the report published in the Proceedings of the Sanibel Symposium /1/, "On Transition Operators for Describing Ionisation and Excitation" has continued in several directions. The main idea is to construct model operators for ionisation and excitation which include "relaxation effects". These have to do with the difference in mean fields between initial and final states. The tool in transition operator theory is an effective Fock operator which, insofar the occupation numbers involved, is half-way between the initial and final state. Further differences from initial and final states are associated to the self-consistency condition inherent to this transition operator. Slater's "Transition state" is related no doubt to this theory, but it perhaps emphasizes too much the presence of an underlying state which is unphysical and fictitious. Liberman's construction relating the ionisation energy to the Koopmans' (unrelaxed) energies of initial and final states is, of course, accurate. The disadvantage is that two calculations are needed and as foundation of potential models it is not entirely satisfactory. This can be seen from the results obtained in connection with the successful parametrisation of electron binding and Auger energies. The results obtained can be surveyed from the bibliography. The first article has been grant supported.

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- P.G. Ellis and O. Goscinski: "Transition State Calculation of Oscillator Strengths in the Local Exchange Approximation", Physica Scripta 9, 104 (1974).
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- H. Siegbahn, R. Medeiros and O. Goscinski: "Direct Calculation of Core Electron Ionisation and Relaxation Energy Using Transition Potentials Applications to Boron Compounds", J. Electron Spectroscopy (1975).
- H. Siegbahn and O. Goscinski: "Transition Potential Models for Auger Electron Spectra" (to be published).

IV. COMPUTATIONAL METHODS FOR ABSORPTION AND MAGNETIC CIRCULAR DICHROISM INTENSITIES

Dennis Caldwell

An analysis of computational methods for absorption and magnetic circular dichroism intensities has been undertaken, beginning with the CNDO/2 method applied to the derivatives of benzene. It has been found that the trends in frequency shifts and intensities can be summarized by a relatively simple and intelligible model:

- 1) The Hartree-Fock energy matrix h_{ij}^F for a given derivative is first locally diagonalized for the chromophore (in this case benzene) leading to determinantal functions with the parent D_{6h} symmetry B_{1u} , B_{2u} , E_{1u} . For example, if h_{ij}^F is expressed in terms of local atomic orbitals after the final iteration, but prior to diagonalization, the matrix element for a ring carbon atom π -orbital is given in atomic units by

$$H_{11} = -.20872,$$

while that for adjacent carbon atoms is given by

$$H_{12} = -.31135.$$

For toluene these same quantities vary slightly from one ring carbon to the next around mean values given by

$$\bar{H}_{11} = -.20914, \quad \bar{H}_{12} = -.31080,$$

while for aniline the values are

$$\bar{H}_{11} = -.21232, \quad \bar{H}_{12} = -.30956.$$

- 2) The energies associated with the D_{6h} LCAO molecular orbitals on the benzene ring display a similar stability to substitution. On the other hand, the canonical Hartree-Fock orbitals are delocalized among the substituents on the ring with much larger variations in energy. Furthermore, if the B_{1u} , B_{2u} , E_{1u} singlet excited states are considered, there will be no clear cut choice of virtual orbitals, and a number of configurations must be considered followed by a CI calculation.

This process may be considerably shortened by treating the following state functions:

$$\Psi_1(E_{1u}) = \frac{1}{\sqrt{2}} \{ |\chi_1 \bar{\chi}_3| + |\chi_2 \bar{\chi}_4| \}$$

$$\Psi_2(B_{1u}) = \frac{1}{\sqrt{2}} \{ |\chi_1 \bar{\chi}_3| - |\chi_2 \bar{\chi}_4| \}$$

$$\Psi_3(CT) = \begin{cases} |\chi_D \bar{\chi}_3| & \text{Donors} \\ |\chi_1 \bar{\chi}_A| & \text{Acceptors,} \end{cases}$$

where χ_D is an appropriate donor orbital such as the nitrogen π -orbital in aniline and χ_A is an acceptor orbital such as the $-\text{NO}_2$ π^* in nitrobenzene. These orbitals are determined by locally diagonalizing the Hartree-Fock Hamiltonian matrix for the groups in question.

A complete treatment of configuration interaction by this method is mathematically equivalent to a CI calculation based on the delocalized Hartree-Fock orbitals with the net result that there is a great tendency to relocalize the electrons on their respective groups. The fact that they are not completely localized is, of course, responsible for the anomalous spectroscopic properties of these derivatives. Furthermore the direct CI method allows a more intimate study of computational quantum mechanics from the chemical standpoint.

- 3) The essential features of larger scale CI calculations can be summarized by a 3×3 determinant, though the precision is not the same:

$$\begin{bmatrix} E_{E_{1u}} & 0 & S_{E_{1u}} \\ 0 & E_{B_{1u}} & S_{B_{1u}} \\ S_{E_{1u}} & S_{B_{1u}} & E_{CT} \end{bmatrix}$$

Here a transition with Y-polarization has been considered, whereby the B_{1u} band borrows from the E_{1u} by mixing with the charge transfer configuration, as described above. The matrix elements, $S_{E_{1u}}$ and $S_{B_{1u}}$, are readily obtained from the localized Hartree-Fock matrix given by the program and the results all scaled to the intensity of the benzene E_{1u} transition.

- 4) The results of this analysis may be summarized as follows:
- a) Frequencies of the transitions are shifted downward by a few per cent.
 - b) The B_{1u} state is shifted away from the E_{1u} .
 - c) The E_{1u} intensities are decreased by 50-75% for strong donors and acceptors.
 - d) The B_{2u} absorption is about 1/10 that of the E_{1u} and that of the B_{1u} is about double the B_{2u} intensity.
 - e) The MCD of the B_{1u} and B_{2u} transitions is increased at the expense of the E_{1u} .
 - f) The signs of the MCD bands for all three transitions are generally reversed for strong acceptor groups like $-NO_2$.
 - g) The sign of the donor tends to be favored in the MCD of para disubstituted Donor-Acceptor derivatives such as nitroaniline.

It is planned to extend this work to a more comprehensive SCF-CI ab initio calculation in order to further delineate the relationship of quantum computational to chemical concepts.

The preliminary conclusion seems to be: If electron densities were not in some way approximately transferable for similar environments, there would be no chemistry; while if they were literally transferable, there would be no interesting chemistry.